Effect of Quantum Confinement on Electron Tunneling through a Quantum Dot

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Abstract

Employing the Anderson impurity model, we study tunneling properties through an ideal quantum dot near the conductance minima. Considering the Coulomb blockade and the quantum confinement on an equal footing, we have obtained current contributions from various types of tunneling processes; inelastic cotunneling, elastic cotunneling, and resonant tunneling of thermally activated electrons. We have found that the inelastic cotunneling is suppressed in the quantum confinement limit, and thus the conductance near its minima is determined by the elastic cotunneling at low temperature ($k_BT \ll \Gamma$, Γ: dot-reservoir coupling constant), or by the resonant tunneling of single electrons at high temperature ($k_BT \gg \Gamma$).
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During last decade, there has been a rapid advance in the field of single electronics, and accordingly much scientific attention has been given to transport properties through ultra-small tunnel junctions such as GaAs quantum dot [1–3]. In a quantum dot with small capacitance, "Coulomb blockade" of tunneling occurs for small bias voltage V when the charging energy (Coulomb energy U) in the dot is sufficiently large as compared to a thermal energy $k_B T$. It occurs because even a single tunneling event increases the electrostatic Coulomb energy of the system considerably. However, even in this regime, a finite current can flow via virtual intermediate states arising from the quantum fluctuation of macroscopic electric charge in the central electrode of the system. This process in a quantum dot, so called cotunneling or macroscopic-quantum-tunneling, was first pointed out by Averin and coworkers [4], and is considered as setting a limit to the performance accuracy of the single electron transistor. They have shown that the transport near conductance minima is dominated by the inelastic cotunneling process involving the creation of an electron-hole excitation in the central electrode, and predicted an algebraic variation of the leakage current with applied voltage ($\sim V^3$) and temperature ($\sim T^2$). The theory of cotunneling has been derived within the lowest order perturbation when the energy discreteness in a quantum dot is not important, *i.e.* the continuous energy spectrum is assumed in the central electrode. The inelastic cotunneling has been observed both in metal-insulator-metal tunnel junctions [5,6] and in a 2D electron system of GaAs/Ga(Al)As heterostructure [7,8].

When dealing with an ultra-small quantum dot, the effect of level discreteness (energy quantization: Δ) becomes very important. The effect will be more prominent in semiconductor systems than in metallic systems, due to much lower electron concentration (ρ) and lower effective electron mass (m^*) in semiconductor systems (recall that a free electron approximation yields $\Delta = \frac{1}{g(\varepsilon_F)V} = \frac{2\hbar^2 \pi^2}{V m^* (3\pi^2 \rho)^{1/3}}$ for 3D systems). There have been quite a few experimental evidences exhibiting coexistence of the charge and energy quantization in the tunneling properties [3]. Furthermore, it is shown that the level spacing Δ can be even comparable to the Coulomb energy U for a Si-based quantum dot transistor [9]. For such systems, the "quantum confinement" will become significant as much as the Coulomb

blockade for the tunneling in the single electron transistor. This kind of electronic confinement could be realized for an ultra-small dot at relatively high temperature. Illustrating typical parameters, a Si dot with diameter of 20nm would have $\Delta \sim 25$ meV, and then the confinement of electron could be realized even at $T < \mathcal{O}(100)$K for $U \sim 15$ meV [9].

We address in this paper whether the inelastic cotunneling phenomenon is really a limiting factor in operating single electron quantum dot devices. For this purpose, we have examined tunneling properties of an ideal quantum dot coupled to two reservoirs in terms of the Anderson impurity model, where the quantum confinement is important as much as the Coulomb blockade. Special attention is focused on the temperature dependence of the inelastic cotunneling by treating the Coulomb blockade and the quantum confinement on an equal footing. We have found that the characteristic of the tunneling in the quantum confined system far from conductance maxima is qualitatively different from the case where the level discreteness can be neglected. In this case, the "inelastic" cotunneling is substantially suppressed at low temperature, while the "elastic" cotunneling or the resonant single electron tunneling of thermally activated electrons dominates in the system. Therefore it is expected that, in small enough quantum dots, there would be no substantial limitation on the performance accuracy in practical devices by a macroscopic quantum tunneling of charge.

We start with the simplest Anderson model Hamiltonian [10] to describe an ideal quantum dot (labeled by D) weakly coupled to two electron reservoirs (labeled by L and R):

$$\mathcal{H} = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_D + \mathcal{H}_T$$

$$\mathcal{H}_{L(R)} = \sum_{k,\alpha \in L(R)} \varepsilon_k c_{k\alpha}^\dagger c_{k\alpha} \tag{1}$$

$$\mathcal{H}_D = \sum_\alpha \varepsilon_\alpha d_\alpha^\dagger d_\alpha + U \sum_{\alpha > \alpha'} n_\alpha n_{\alpha'}$$

$$\mathcal{H}_T = \sum_{k,\alpha \in L,R} \left(V_{k\alpha} c_{k\alpha}^\dagger d_\alpha + \text{h.c.} \right).$$

Here $\mathcal{H}_L, \mathcal{H}_R, \mathcal{H}_D$ and $\mathcal{H}_T$ represent Hamiltonians of the left reservoir, the right reservoir, an interacting dot, and tunneling between the dot and reservoirs, respectively. The levels in

the dot are labeled by an index α, and U denotes the Coulomb interaction between electrons in the dot. The states in the reservoirs with energies ε_k are coupled to the dot by hopping matrix element $V_{k\alpha}$. The transition rate of an electron between the level ε_α and the reservoir $L(R)$ is given by

$$\Gamma_{L(R)}^\alpha(\omega) = 2\pi \sum_{k \in L(R)} |V_{k\alpha}|^2 \, \delta(\omega - \varepsilon_k). \tag{2}$$

This Anderson-type Hamiltonian has been recently employed to describe transport in the quantum dot structure [11–14]. In the Coulomb blockade and the quantum confinement limit, we have

$$U, \Delta \gg k_B T, \Gamma_{L(R)}, eV \tag{3}$$

where eV corresponds to a potential energy difference coming from the bias voltage across two reservoirs.

The cotunneling refers to a simultaneous tunneling of two electrons through intermediate states with an extra electron or hole in a quantum dot. This second order cotunneling process is called "inelastic" if there remains an electron-hole excitation after the process (Fig1.(a)), whereas the process is said to be "elastic" if no electron-hole excitation is left (Fig1.(b)). The inelastic cotunneling current can be simply calculated by using the Fermi golden rule.

The initial eigenstate $|I\rangle$ of the Hamiltonian $\mathcal{H}_0 = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_D$ can be written as $|\phi_L\rangle|\psi^N\rangle|\phi_R\rangle$, where $|\phi_{L(R)}\rangle$ denotes the Fermi sea of left (right) reservoirs, and $|\psi^N\rangle$ represents an N-particle eigenstate of $\mathcal{H}_D$. There are two kinds of final states for inelastic cotunneling processes. Those are $|F_1\rangle$ (an electron(hole) tunnels from $L(R)$ to $R(L)$), and $|F_2\rangle$ (an electron(hole) tunnels from $R(L)$ to $L(R)$), such that $|F_1\rangle = c_{p\beta}^\dagger d_\beta d_\alpha^\dagger c_{k\alpha}|I\rangle$, $|F_2\rangle = c_{k\alpha}^\dagger d_\alpha d_\beta^\dagger c_{p\beta}|I\rangle$ ($k \in L, p \in R$). The inelastic cotunneling yields the current as

$$I^{in}(V) = e\left(\gamma_1(V) - \gamma_2(V)\right), \tag{4}$$

where γ_1 and γ_2 are statistical averages of the transition rates from the initial state $\{|I\rangle\}$ to the final states $\{|F_1\rangle\}$ and $\{|F_2\rangle\}$, respectively, and are expressed as

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$$\gamma_i = \left\langle \frac{2\pi}{\hbar} \sum_{F_i} |\langle I| \mathcal{H}_T \frac{1}{E_I - \mathcal{H}_0} \mathcal{H}_T |F_i\rangle|^2 \delta(E_I - E_{F_i}) \right\rangle_I \quad i = 1, 2, \tag{5}$$

with $\langle \cdots \rangle_I$ denoting the statistical average over the initial states.

For a constant $\Gamma_{L(R)} = \Gamma^\alpha_{L(R)}(\varepsilon)$, γ_1, γ_2 are given by

$$\gamma_1(V) = \frac{\Gamma_L \Gamma_R}{h} \sum_{\alpha \neq \beta} \langle n_\beta(1 - n_\alpha) \rangle \int d\varepsilon d\varepsilon' f(\varepsilon)(1 - f(\varepsilon'))$$

$$\times \left(\frac{1}{\varepsilon_\alpha - \varepsilon + \mu_a} + \frac{1}{\varepsilon' - \varepsilon_\beta + \mu_b} \right)^2 \delta\left(\varepsilon' - \varepsilon_\beta + \varepsilon_\alpha - \varepsilon - eV\right) \tag{6a}$$

$$\gamma_2(V) = \gamma_1(-V). \tag{6b}$$

Here $\langle \cdots \rangle$ denotes statistical average, and $f(\varepsilon) = 1/(e^{\beta\varepsilon} + 1)$ is the Fermi distribution function for the reservoirs. $\mu_a(\mu_b)$ represents the charging energy of the virtual intermediate state with one extra electron (hole). They are defined by

$$\mu_a = NU - \mu_L, \tag{7a}$$

$$\mu_b = \mu_R - (N - 1)U, \tag{7b}$$

with $\mu_L(\mu_R)$ being the chemical potential of the left (right) reservoir which satisfies the relation $\mu_L - \mu_R = eV$. Equation (6) describes well the inelastic cotunneling when the system is not too close to the conductance maxima.

Note that, if one assumes a continuous spectra for electrons in the dot ($\Delta \to 0$), Eq.(6) becomes equivalent to the result by Averin and Nazarov [4], since then $\langle n_\beta(1 - n_\alpha) \rangle = f_\beta(1 - f_\alpha)$ with f being the Fermi distribution function. However, in the quantum confinement limit, the inelastic cotunneling process described by Eq.(6) gives rise to drastically modified characteristics due to following two reasons. First, for the electrons in the dot, the Fermi distribution function cannot be used in the quantum confinement limit ($k_B T, eV \ll \Delta$), because the number fluctuation is very small [15,16]. Second, more important difference results from the fact that there is no available excitation for inelastic cotunneling process with energy ε such that $0 < \varepsilon < \Delta$. Therefore it is expected that the inelastic cotunneling rate is much suppressed in the quantum confinement limit.

To see the functional form of the inelastic cotunneling current in the quantum confinement limit, it will be sufficient to consider lowest two levels. It is because contributions from other levels would be exponentially small as compared to those of two levels. Let's assign the two levels as $\varepsilon_1 = 0$ and $\varepsilon_2 = \Delta$ with $N = 1$ for the ground state of the dot. Then we have $\langle n_1 n_2 \rangle = 0$, and Eq.(6) reduces to

$$
\begin{aligned}
\gamma_1(V) = \frac{\Gamma_L \Gamma_R}{h} \int & d\varepsilon\, f(\varepsilon)(1 - f(\varepsilon')) \\
\times & \left[\langle n_1 \rangle \left(\frac{1}{\Delta - \varepsilon + \mu_a} + \frac{1}{\varepsilon' + \mu_b} \right)^2 \delta\left(\varepsilon' - \varepsilon + \Delta - eV\right) \right. \\
& \left. + \langle n_2 \rangle \left(\frac{1}{-\varepsilon + \mu_a} + \frac{1}{\varepsilon' - \Delta + \mu_b} \right)^2 \delta\left(\varepsilon' - \varepsilon - \Delta - eV\right) \right].
\end{aligned}
\tag{8}
$$

Here $\langle n_1 \rangle = 1/(1 + e^{-\beta\Delta})$ and $\langle n_2 \rangle = e^{-\beta\Delta}/(1 + e^{-\beta\Delta})$. The first(second) term in Eq.(8) describes the excitation (relaxation) process from initially ground (excited) state in the dot. Further, in the quantum confinement limit, $\langle n_2 \rangle$ is exponentially small, and so a contribution from the second term can be neglected. Then using $\langle n_1 \rangle \simeq 1$, Eq.(8) becomes

$$
\gamma_1(V) \simeq \frac{\Gamma_L \Gamma_R}{h} \int d\varepsilon\, f(\varepsilon) f(\Delta - eV - \varepsilon) \left(\frac{1}{\Delta - \varepsilon + \mu_a} + \frac{1}{\varepsilon - \Delta + eV + \mu_b} \right)^2.
\tag{9}
$$

Since $f(\varepsilon)f(\Delta - eV - \varepsilon)$ is peaked around $\varepsilon \sim \Delta/2$, Eq. (9) is approximated by

$$
\begin{aligned}
\gamma_1(V) &\simeq \frac{\Gamma_L \Gamma_R}{h} \left(\frac{1}{\mu_a + \Delta/2} + \frac{1}{\mu_b - \Delta/2} \right)^2 \int d\varepsilon\, f(\varepsilon) f(\Delta - eV - \varepsilon) \\
&\simeq \frac{\Gamma_L \Gamma_R}{h} \left(\frac{1}{\mu_a + \Delta/2} + \frac{1}{\mu_b - \Delta/2} \right)^2 (\Delta - eV)\, e^{\beta eV} e^{-\beta\Delta}.
\end{aligned}
\tag{10}
$$

Notable in Eq. (10) is that the inelastic cotunneling current in the quantum confinement limit has a temperature dependence $e^{-\beta\Delta}$ suggesting very much suppression at low temperature. This is in contrast to T^2-dependence Averin and Nazarov have obtained for $\Delta \to 0$ limit [4]. The suppression of the inelastic cotunneling in the quantum confinement limit originates from the reduction of phase space for the electron-hole excitations in the dot. Hence, in this limit, other kinds of processes such as elastic cotunneling or single electron tunneling of thermally activated electrons is expected to determine conductance minima [17].

The contributions from the elastic cotunneling and the single electron tunneling of thermally activated electrons can be estimated by Landauer-type formula through an interacting region [18]. For the Anderson Hamiltonian, the conductance takes the following form in the linear response regime,

$$G = \frac{e^2}{\hbar}\tilde{\Gamma}\int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right)\sum_\alpha \rho_\alpha(\varepsilon), \tag{11}$$

where $\tilde{\Gamma} = \frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}$, $f(\varepsilon) = 1/(e^{\beta(\varepsilon-\mu)}+1)$ $(\mu = \mu_L = \mu_R)$, and $\rho_\alpha(\varepsilon) = -\frac{1}{\pi}\mathrm{Im}G_\alpha(\varepsilon)$ is local density of states of electrons with label α. Equation of motion - decoupling method can be used to get an approximate solution of the Green's function G_α [12,19]. In the present study, more subtle Kondo effect will not be taken into account [13,14]. Then Green's functions can be expressed as

$$G_1(\varepsilon) \sim \frac{1}{\varepsilon + i\Gamma/2}, \quad G_2(\varepsilon) \sim \frac{1}{\varepsilon - (\Delta + U) + i\Gamma/2}, \tag{12}$$

where $\Gamma = \Gamma_L + \Gamma_R$.

The conductance near its minima shows a different feature depending on the relative size of Γ and k_BT. For $\Gamma \gg k_BT$, $\left(-\frac{\partial f}{\partial \varepsilon}\right)$ in Eq. (11) can be approximated by $\delta(\varepsilon - \mu)$ and the elastic cotunneling dominates (Fig1.(b)):

$$G \simeq \frac{e^2\Gamma_L\Gamma_R}{h}\left(\frac{1}{\mu^2} + \frac{1}{(\Delta + U - \mu)^2}\right). \tag{13}$$

On the other hand, for $\Gamma \ll k_BT$, there appears a limit in which the 'resonant' tunneling of thermally activated electrons (Fig1.(c)) becomes most important. In this case, $\rho_1(\varepsilon) \simeq \delta(\varepsilon), \rho_2(\varepsilon) \simeq \delta(\varepsilon - \Delta - U)$, and thus we have

$$G \simeq \frac{e\tilde{\Gamma}}{\hbar}\left[-f'(0) - f'(\Delta + U)\right]. \tag{14}$$

In any case, the inelastic cotunneling process has much smaller contribution to the conductance than other processes. Present results can be summarized as in Fig. 2, which shows a schematic diagram of off-resonance tunneling processes. We have examined tunneling properties in the quantum confinement regime $(T/\Delta \ll 1)$, in which the elastic cotunneling (A)

or the resonant tunneling (B) is dominating. Note that the inelastic cotunneling (C), which has been dealt with in previous studies [4], becomes significant only in the opposite limit $(T/\Delta \gg 1)$.

In conclusion, we have analyzed off-resonance tunneling properties of an ideal quantum dot coupled to two reservoirs, in terms of the Anderson impurity model. We have found that, in the quantum confinement limit, the inelastic cotunneling of electrons is much suppressed, which is contrary to the case of previously studied $\Delta \to 0$ limit. The suppression of the inelastic cotunneling current originates from the absence of phase space for the electron-hole excitations in the dot with energy ε such that $0 < \varepsilon < \Delta$. Hence, near the conductance minima, the transport is governed by the elastic cotunneling or by the resonant tunneling of thermally activated electrons. The present result strongly suggests that the usually thought performance limitation of single electron devices arising from the inelastic cotunneling phenomena would be considerably reduced in an ultra-small quantum dot at sufficiently low temperature.
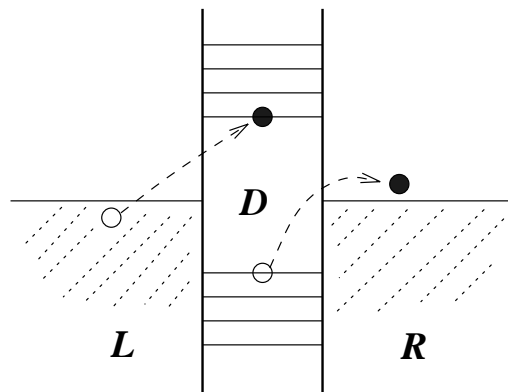
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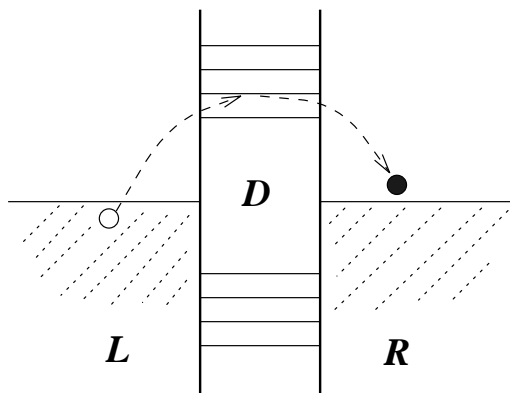[19] K. Kang and B. I. Min, Phys. Rev. B **52**, 10689 (1995).

FIGURES

FIG. 1. Various types of electron tunneling processes near conductance minima; (a) inelastic cotunneling, (b) elastic cotunneling, and (c) resonant tunneling of thermally activated electron.
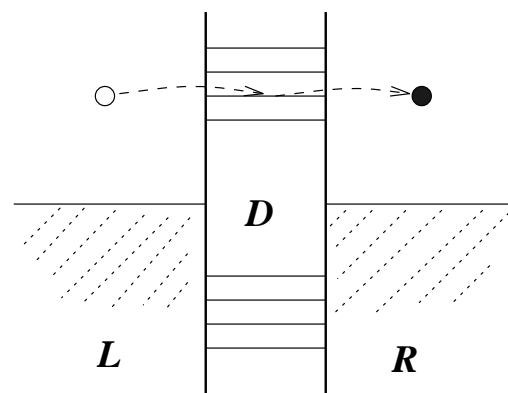
FIG. 2. Schematic diagram of showing various off-resonance tunneling processes for different regimes defined by the ratios T/Δ and Γ/Δ. A, B, and C correspond to regions in which tunneling processes of the elastic cotunneling, the resonant tunneling of activated electrons, and the inelastic cotunneling are dominating, respectively. The Coulomb blockade limit $U \gg kT$ is being considered here.
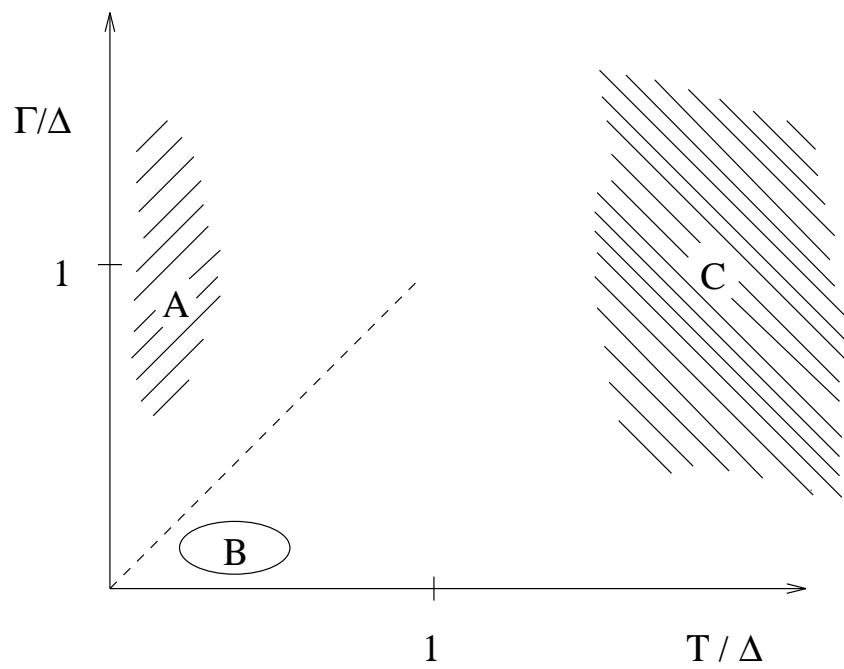
(a)

(b)   (c)

Fig. 1

Fig. 2